CORRESPONDENCE

Comments on "The Over-Relaxation Factor in the Numerical Solution of the Omega Equation"

JAMES J. O'BRIEN

National Center for Atmospheric Research, Boulder, Colo.

1. INTRODUCTION

The recent paper by Stuart and O'Neill [4] is concerned with determining the optimum over-relaxation coefficient in the numerical relaxation of the omega equation. These authors do not consider some well-known theoretical aspects of iteration procedures. At least, from the pedagogic point of view, it is instructive to reanalyze their problem.

They consider the omega equation in the form

$$B(p)\nabla_p^2\omega + \frac{\partial^2\omega}{\partial p^2} = G(x, y, p). \tag{1}$$

The application of centered differences to (1) yields the finite difference form:

$$\omega_{i,j+1,p} + \omega_{i+1,j,p} + \omega_{i,j-1,p} + \omega_{i-1,j,p} - K'_{ijp} \omega_{ijp} + K_{ijp} [\omega_{i,j,p+\Delta_p} + \omega_{i,j,p-\Delta_p}] = L_{ijp}, \quad (2)$$

where

$$K_{ijp} = \frac{a^2}{m^2 B(p) (\Delta p)^2}$$

$$K'_{ijn} = 4 + 2K_{ijn}$$

$$L_{ijp} = \frac{a^2}{m^2 B(p)} G_{ijp}$$
.

The horizontal grid size is $a=\Delta x=\Delta y$; Δp is the vertical grid interval and m is map factor, taken to be unity. Equation (2) is the complete three-dimensional equation. Stuart and O'Neill also consider the special two-dimensional case, $K_{ijp}=0$, and the one-dimensional equation, B(p)=0, whose finite difference form is

$$\omega_{i,j,p+\Delta p} - 2\omega_{i,j,p} + \omega_{i,j,p-\Delta p} = (\Delta p)^2 G_{ijp}. \tag{3}$$

Note the minus sign is a correction of a misprint from the original paper. The subscripts i,j can be dropped from (3) without any loss of generality.

If the left-hand side of (1) or (3) is denoted $\Gamma(\omega)$, a residual, R^N , may be defined

$$R^{N} = \Gamma(\omega^{N}) - L_{tin}, \tag{4}$$

where N is the number of scans in the iteration procedure. This notation is misleading since R is dependent, in actual application, on N and N+1, as we shall see.

The relaxation technique consists of correcting each ω using the relation

$$\omega^{N+1} = \omega^N + \alpha R^N, \tag{5}$$

which is assumed to be valid for every point (i,j,p); α is the over-relaxation factor. In practice, the initial guess ω^0 is zero for all ω . Note that (5) is linear in ω_{ijp} .

At this point it is necessary to leave the discussion of the numerical solution of the omega equation and recall some theorems concerning the iterative solution of linear equations. Faddeeva [2] is an excellent source for this discussion. Let us consider a set of n linear equations in the form

$$X = AX + F, \tag{6}$$

where A is the matrix of coefficients, \mathbb{F} the column matrix or vector of constants, and \mathbb{X} the column matrix of n unknowns. The Gauss-Jacoby or Ordinary Process of Iteration consists of writing (6) as

$$X^{(k+1)} = AX^{(k)} + \mathbb{F}. \tag{7}$$

which in an explicit form we mean

$$x_i^{(k+1)} = \sum_{j=1}^{n} a_{ij} x_j^{(k)} + f_i.$$
 (8)

The process of iteration consists of choosing a certain vector $\mathbb{X}^{(0)}$ and finding $\mathbb{X}^{(1)}$, $\mathbb{X}^{(2)}$, etc., until for a preassigned ϵ_t

$$|x_i^{(k+1)}-x_i^{(k)}|<\epsilon_i$$
 for all i .

Faddeeva gives us the fundamental theorem: For convergence of the process of iteration with any initial vector $\mathbb{X}^{(0)}$ and with any value of the vector \mathbb{F} , it is necessary and sufficient that all eigenvalues of the matrix \mathbb{A} be less than unity in modulus. This theorem is quite important and the proof is given by Faddeeva.

The Gauss-Seidel iterative method is similar to the ordinary iterative process except that in computing the

(k+1) approximation to x_i , one takes into consideration the (k+1)th approximations already computed to the components $x_1, x_2, \ldots x_{i-1}$. Equation (8) is written for the Gauss-Seidel method

$$x_i^{(k+1)} = \sum_{j=1}^{i-1} a_{ij} x_j^{(k+1)} + \sum_{j=i}^{n} a_{ij} x_j^{(k)} + f_i; \qquad i=1, 2, \dots, n. \quad (9)$$

Let us write the equation (6) in the form

$$X = (\mathbb{B} + \mathbb{C})X + \mathbb{F}, \tag{10}$$

where the only non-zero elements of \mathbb{B} are the elements a_{ij} below the main diagonal and \mathbb{C} contains as non-zero elements the diagonal elements a_{ii} and the elements a_{ij} above the main diagonal. Using these definitions for \mathbb{B} and \mathbb{C} , the Gauss-Seidel process (9) becomes

$$\mathbb{X}^{(k+1)} = \mathbb{B}\mathbb{X}^{(k+1)} + \mathbb{C}\mathbb{X}^{(k)} + \mathbb{F},\tag{11}$$

or, rearranging.

$$\mathbb{X}^{(k+1)} = (\mathbb{I} - \mathbb{B})^{-1} [\mathbb{C} \mathbb{X}^{(k)} + \mathbb{F}] = \mathbb{M} \mathbb{X}^{(k)} + \mathbb{G}. \tag{12}$$

Hence the Gauss-Seidel method, (11), is equivalent to applying the ordinary process of iteration to (12) where \mathbb{M} plays the role of the matrix \mathbb{A} in the fundamental theorem and $\mathbb{G} = (\mathbb{I} - \mathbb{B})^{-1}\mathbb{F}$.

Using this background and the well-known fact (e.g. Varga [5]) that the speed of convergence is directly dependent on the spectral radius, i.e., the absolute value of maximum eigenvalue of A or M as applicable to a particular case, we now return to the over-relaxation of the omega equation as considered by Stuart and O'Neill. First we shall consider the one-dimensional case, then the two-dimensional case and, finally, the three-dimensional case.

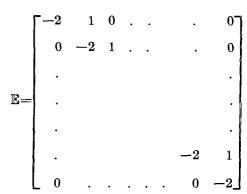
2. ONE-DIMENSIONAL CASE

The insertion of equation (3) in (4) yields

$$\mathbb{W}^{(k+1)} = \mathbb{W}^{(k)} + \alpha [\mathbb{D}\mathbb{W}^{(k+1)} + \mathbb{E}\mathbb{W}^{(k)} - \mathbb{L}], \tag{13}$$

where $\dot{\mathbb{W}}^T = [\omega_1, \ \omega_2, \ \omega_3, \ \dots \ \omega_l]$ (read \mathbb{W}^T as transpose of \mathbb{W}). We are considering an arbitrary number of levels, l, at which omega is to be determined. The matrices \mathbb{D} and \mathbb{E} are of order l and have the form

$$\mathbb{D} = \begin{bmatrix} 0 & 0 & \dots & \dots & 0 \\ 1 & 0 & & & \dots \\ 0 & 1 & & & \dots \\ \vdots & & & \ddots & & \vdots \\ \vdots & & & & \ddots & \vdots \\ 0 & & & & 1 & 0 \end{bmatrix}$$



We can only presuppose that (13) represents the process used by Stuart and O'Neill under the additional empirical requirement that $\alpha=0$ when $|\mathbf{R}^N| \leq \epsilon$, where ϵ is their present tolerance. This empirical alteration to the usual extrapolated Leibmann relaxation scheme leads to a difficulty in performing an exact theoretical analysis. Here we assume that the correction, \mathbf{R}^N , is applied even though $|\mathbf{R}^N| < \epsilon$ for some ω_i . As a principle of faith, we, intuitively, believe that the theoretical analysis is applicable to the approximation scheme. Stuart and O'Neill state that there is no difference in their results for the cutoff and optimum value of the over-relaxation parameter, α , as compared to other estimates, and this strengthens our supposition.

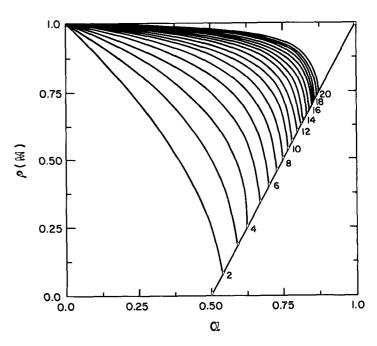


FIGURE 1.—Spectral radius, $\rho(\mathbb{M})$, as a function of the over-relaxation coefficient, α , for the 1-D omega equation. The line from 0.5 to 1 is common to all curves. The value of the number of levels, l, for l=2(1)20 specifies the appropriate curve.

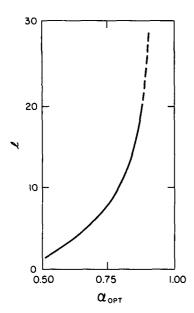


FIGURE 2.—The number of levels, l, as a function of the optimum over-relaxation coefficient, α_{opt} , with l=1(1)20 for the 1-D case. As $l\to\infty$, α_{opt} must approach 1.0.

We now consider α to be specified and note that (13) is equivalent to (11) if

$$X=W$$
 $B=\alpha D$
 $C=I+\alpha E$
 $F=-\alpha L$.

Thus, the convergence of (13) depends on the spectral radius of

$$M = (I - B)^{-1}C = (I - \alpha D)^{-1}(I + \alpha E).$$
 (14)

The cutoff α 's, i.e., the allowable bounds on α for convergence, are determined by finding the values of α which permit the spectral radius of \mathbf{M} , $\rho(\mathbf{M})$, to be 1 and -1. A routine analysis shows that, in this simple case, $0 < \alpha < 1$ restricts $|\rho(\mathbf{M})| \le 1$. The two-dimensional case and the three-dimensional case are not easily analyzed by hand. In this simple case, the allowable range of α is not dependent on l, the number of levels and indeed, as we shall see, this conclusion follows for the 2-D case also.

The determination of the optimum value of ω requires more ingenuity. The suggested procedure is to specify $0 < \omega < 1$ and determine $\rho(\mathbf{M})$ and, thus, find the value of ω which minimizes $\rho(\mathbf{M})$. In brief, α was specified between 0 and 1 and l was allowed to vary from 2 to 20. Figure 1 was constructed from the computer results. The case l=4 corresponds to the six-level model of Stuart and O'Neill. The optimum α is 0.63. Figure 2 shows the optimum α (α_{opt}) as a function of l. Stuart and O'Neill conclude that "the optimum α for the 1-D equation would probably show only slight variations from one grid to another." This conclusion is very misleading.

Figure 2 shows the effect of the number of levels, l, on α_{opt} ; as l increases α_{opt} approaches 1.0.

Note, since the convergence of (11) is independent of \mathbf{F} and $\mathbf{X}^{(0)}$, the convergence of the physical problem (13) is independent of $L_p = (\Delta p)^2$ G_{ijp} and the initial guess, $\mathbf{W}^{(0)}$. Since the omega equation is linear, we should not be surprised that convergence is independent of the forcing function or the initial guess. However, in general, we shall see that the optimum omega will depend on the number of grid points and, in the 3-dimensional case, on other physical parameters. Naturally, the number of iterations required should be dependent on our initial guess, $\mathbf{W}^{(0)}$, since if the process will converge with a particular choice of α , then a "close guess" to the desired \mathbf{W} will result in rapid convergence. But for arbitrary α , the speed of convergence should only be related to $\rho(\mathbf{M})$.

3. TWO-DIMENSIONAL CASE

The omega equation becomes

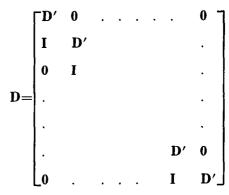
$$\nabla_{\mathbf{p}}^{2}\omega = G(x, y, p)/B(\mathbf{p}). \tag{15}$$

The centered finite difference equation in matrix form for over-relaxation is

$$\mathbf{W}^{(k+1)} = \mathbf{W}^{(k)} + \alpha [\mathbf{D}\mathbf{W}^{(k+1)} + \mathbf{E}\mathbf{W}^{(k)} - \mathbf{L}]. \tag{16}$$

where $\mathbf{W}^T = [\omega_{11}, \omega_{12}, \ldots, \omega_{1n}, \omega_{21}, \omega_{22}, \ldots, \omega_{2n}, \ldots, \omega_{rn}]$. There are other orders which are allowable, e.g., see Fox [3] for a discussion of this aspect of the problem. The special case $\Delta x = \Delta y = a$ is considered and there are $n \times r$ total points on a particular rectangular pressure surface.

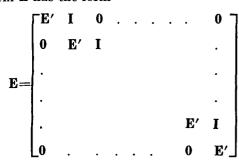
D is of order $r \times n$ and has the form



where D', 0, I are square matrices of order n. I is the identity matrix, 0 is the null matrix and

$$\mathbf{D}' = \begin{bmatrix} 0 & 0 & \dots & \dots & 0 \\ 1 & 0 & & & \dots \\ 0 & 1 & & & & \dots \\ \vdots & & & & \ddots & \vdots \\ 0 & 0 & \dots & \dots & 1 & 0 \end{bmatrix}$$

The matrix E has the form



where E', I, 0 are square matrices of order n and

$$\mathbf{E'} = \begin{bmatrix} -4 & 1 & 0 & \dots & 0 \\ 0 & -4 & 1 & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & &$$

 $\mathbf{L} = (a^2/B(p)) [g_{i,j,p}] \text{ and } g_{i,j,p} \text{ is an element of } \mathbf{G}_{i,j,p}.$

The over-relaxation scheme for (16) is similar to the Gauss-Seidel method given by (11) if we equate

$$X = W$$

$$B = \alpha D$$

$$C = I + \alpha E$$

$$F = -\alpha L$$

Thus, as before, convergence or (16) is dependent only on the spectral radius of

$$\mathbf{M} = (\mathbf{I} - \mathbf{B})^{-1} \mathbf{C} = (\mathbf{I} - \alpha \mathbf{D})^{-1} (\mathbf{I} + \alpha \mathbf{E}). \tag{17}$$

Note, since **D** and **E** are independent of Δx , Δy , **W** and the forcing function, convergence is independent of $\mathbf{W}^{(0)}$, the initial guess, the grid-spacing (when $\Delta x = \Delta y$), and the forcing function.

Now, since we desire to use an over-relaxation scheme, $\alpha > \frac{1}{4}$. Therefore, the cutoff α 's are easily found by allowing α to vary from 0 to 1 and by determining $\rho(\mathbf{M})$, using an available matrix subroutine. The optimum α is found by the above procedure, since as we allow α to take on values [0, 1], $\rho(\mathbf{M})$ will be found also. The minimum value of $\rho(\mathbf{M})$ shall be taken to be related to the optimum α .

Following Stuart and O'Neill, let n=r; i.e., consider only square regions. Look first at the trivial case, n=1 where $\mathbf{M}=1-4\alpha$. Hence $0<\alpha<\frac{1}{2}$ restricts $\rho(\mathbf{M})<1$ and the optimum α is 0.25. From the analysis of Carré [1] and the 1-D case, we expect, as n increases, the cutoffs to remain the same and the optimum α to approach 0.5. Figure 3 was constructed from the computer analysis for n=2(1)10. Note, for n=10, \mathbf{M} is of order 100 and considerable computer storage is required.

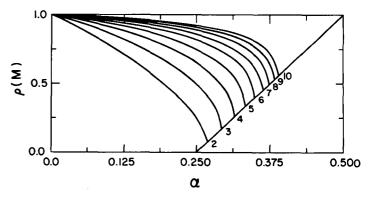


FIGURE 3.—Spectral radius, $\rho(\mathbf{M})$ as a function of the over-relaxation coefficient, α , for the 2-D omega equation. The line from 0.25 to 0.5 is common to all curves. The value of the number of grid points, n, for n=1(1)10 specifies the appropriate curve.

The results for α_{opt} are plotted in figure 4. The curve is extrapolated toward n=20. These results illustrate quite clearly that an understanding of the theory of iterative processes can provide considerable insight for understanding the over-relaxation procedure. For example, the sharp cutoff α found by Stuart and O'Neill is easily explained. We find that α must be less than 0.5 if $\rho(\mathbf{M})$ is to be less than unity for all square grids and the size of the grid, n, is the only free parameter in the analysis. All the other physical parameters do not influence $\rho(\mathbf{M})$. Therefore, if one plots the number of scans versus α , one must find a very sharp cutoff, because the number of scans must approach infinity as $\alpha \rightarrow 0.5$. On any scale, an extremely rapid increase in the number of scans will result.

4. THREE-DIMENSIONAL CASE

The entire problem is a great deal more specialized as we shall see. The combination of equations (2), (4), and (5) leads to the matrix equation

$$\mathbf{W}^{(k+1)} = \mathbf{W}^{(k)} + \alpha [\mathbf{P}\mathbf{W}^{(k+1)} + \mathbf{Q}\mathbf{W}^{(k)} - \mathbf{L}], \tag{18}$$

which is similar to (16) except that

$$\mathbf{W}^{T} = [\omega_{ijp}]^{T} = [\omega_{111}, \omega_{121}, \ldots, \omega_{1n1}, \omega_{211}, \ldots, \omega_{rn1}, \omega_{112}, \ldots, \omega_{rnl}],$$

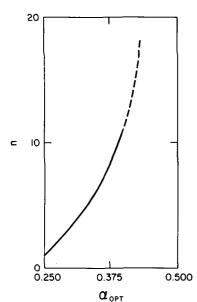


FIGURE 4.—The number of grid points in a square array, n, as a function of the optimum over-relaxation coefficient, α_{opt} , with n=1(1)10 for the 2-D case. As $n\to\infty$, α_{opt} must approach 0.5. Note, the function is extrapolated to n=20 based on Stuart and O'Neill's work.

where **P** and **Q** are of order $n \times r \times l$ and **D** is exactly as that for (16). \mathbf{R}_q is a diagonal matrix

In addition

$$\mathbf{Q} = egin{bmatrix} \mathbf{E}_1 & \mathbf{R}_2 & \mathbf{0} & \dots & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{E}_2 & \mathbf{R}_3 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \mathbf{0} & \dots \end{bmatrix}$$

where $\mathbf{E}_q = \mathbf{E}$ except that the diagonal elements of \mathbf{E}' are $-K'_{ijp}$ instead of -4. \mathbf{R}_q in \mathbf{Q} are as in \mathbf{P} . An element of \mathbf{L} is L_{ijp} .

Rearranging (18) we find

$$\mathbf{W}^{(k+1)} = (\mathbf{I} - \alpha \mathbf{P})^{-1} [(\mathbf{I} + \mathbf{Q}) \mathbf{W}^{(k)} - \mathbf{L}]. \tag{19}$$

Hence, for this problem, $\mathbf{M} = (\mathbf{I} - \alpha \mathbf{P})^{-1}$ $(\mathbf{I} + \mathbf{Q})$; i.e., convergence is assured if $\rho(\mathbf{M}) < 1$. Note, however, in this problem that $\rho(\mathbf{M})$ is a function of α , a, Δp , B(p), and the number of grid points. It is not dependent on the initial guess $\mathbf{W}^{(0)}$, the boundary conditions and the forcing function. For a particular investigation, a, Δp , B(p) and the number of grid points would be specified from physical or economical considerations and, in principle, the optimum value of α can be found by allowing α to vary from 0 to $\frac{1}{2}$ and we can thus find the value of α which minimizes $\rho(\mathbf{M})$.

In this special case, we feel it is not practical to perform an analysis as performed for the 1-D and 2-D cases. The analysis can only be of interest to a few investigators who might choose (1) a square region, (2) the identical profile of σ , (3) the same pressure interval, etc. However, we can offer the following suggestions. First, the work of Carré [1] should be reviewed by all investigators who are interested in this problem. Carré outlines a practical procedure to determine the optimum relaxation coefficient as the numerical solution of an elliptic equation is being accomplished. His techniques are based on a sound theoretical understanding of the iterative process.

Secondly, we must concur with Stuart and O'Neill that the discrepancy between their results and the theoretical results are easily explained by the distinctly different physical problem analyzed by them. Finally, the strange result for the 1.5° grid must be suspect since if we consider the trivial case, n=1, $0<\alpha<2/(4+2K_{ijp})$. Now, since only a is varied, the maximum α must decrease as a increases. This was found for a=1,2,3 degrees, but not for the 1.5-degree case.

5. CONCLUSION

In brief, we have demonstrated the importance of various physical parameters on the convergence of the omega equation in one, two, and three dimensions. It is conceptually possible to analyze the empirical results of Stuart and O'Neill using well-known theoretical aspects of iterative methods for solving systems of linear equations on a computer.

It is recognized that the empirical approach of Stuart and O'Neill may be the most feasible way to determine the optimum over-relaxation coefficient. However, this practical attack must be tempered with a knowledge of the theoretical basis of iterative processes. Such a blend is outlined by Carré [1].

ACKNOWLEDGMENTS

The work of Stuart and O'Neill was brought to my attention while I was a Visiting Lecturer at the Department of Meteorology, Florida State University, during the summer of 1967. The necessary programing was performed by John Liu on his brief visit to the NCAR Computing Center in 1967.

REFERENCES

- B. A. Carré, "The Determination of the Optimum Accelerating Factor for Successive Over-Relaxation," Computer Journal, vol. 4, No. 1, Apr. 1961, pp. 73-78.
- V. N. Faddeeva, Computational Methods of Linear Algebra, Dover Publications, New York, 1959, 252 pp.
- 3. L. Fox, Numerical Solution of Ordinary and Partial Differential Equations, Pergamon Press, Oxford, 1962, 509 pp.
- W. Stuart and T. H. R. O'Neill, "The Over-Relaxation Factor in the Numerical Solution of the Omega Equation," Monthly Weather Review, vol. 95, No. 5, May 1967, pp. 303-307.
- R. S. Varga, Matrix Iterative Analysis, Prentice-Hall, Englewood Cliffs, N.J., 1962, 322 pp.

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Reply

DAVID W. STUART

Florida State University, Tallahassee, Fla.

We are indebted to Dr. O'Brien [1] for calling the work of Carré [2] to the attention of us and perhaps of other investigators. Our interest in the omega equation stems from a desire to use this equation to obtain diagnostic vertical motions for careful analysis of the three-dimensional structure of atmospheric systems. Having started such studies late in 1960 prior to the work of Carré and prior to knowledge of Miyakoda's [3] work, I was forced into the more empirical approach for finding the optimum over-relaxation factor, α_{ont} , as mentioned in our paper (Stuart and O'Neill [4]). Since some knowledge of the over-relaxation factor was needed for our work, we decided to search a bit for α_{opt} . We tested the 1-D and 2-D cases more for completeness and to show that our relaxation technique fitted the known theoretical results. Suffice it to say that our paper reports on the results of an α_{opt} study for a particular grid and stability profile and we hope other investigators will benefit by Carré's paper and our results. Indeed we have followed the approach suggested by O'Brien at the end of his section 4, but without the aid of Carré's work.

Recently I have extended the model to yield omega at nine interior levels for the 2° grid (i.e., $N_x = N_y = 18$, $N_p = 11$, $\Delta p = 10$ cb., and σ for the standard atmosphere). $\alpha_{opt} = 0.15$ was found with the sharp cutoff near 0.20. Again α_{opt} was found at a much lower value than the 0.33 given by Miyakoda's [3]. It is hoped that the results for α_{opt} obtained for our grid model will be of aid to others using very similar models for obtaining omega.

REFERENCES

- J. J. O'Brien, "On the Over-Relaxation Factor in the Numerical Solution of the Omega Equation," Monthly Weather Review, vol. 96, No. 2, Feb. 1968, pp. 99-104.
- B. A. Carré, "The Determination of the Optimum Accelerating Factor for Successive Over-Relaxation," Computer Journal, vol. 4, No. 1, Apr. 1961, pp. 73-78.
- 3. K. Miyakoda, "Test of Convergence Speed of Iterative Methods for Solving 2 and 3 Dimensional Elliptic-Type Differential Equations," Journal of the Meteorological Society of Japan, Ser. 2, vol. 38, No. 2, Apr. 1960, pp. 107-124.
- 4. D. W. Stuart and T. H. R. O'Neill, "The Over-Relaxation Factor in the Numerical Solution of the Omega Equation," Monthly Weather Review, vol. 95, No. 5, May 1967, pp. 303-307.

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